2-Amino-5-methylbenzenesulfonic acid

88-44-8 | DTXSID7026526

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 310 °C

Global applicability domain: Outside

Local applicability domain index: 1.95e-01

Confidence level: 5.80e-01

Nearest Neighbors from the Training Set

Image not found
Chloramben
Measured: 312
Predicted: 301

Image not found
Trimellitic anhydride
Measured: 390
Predicted: 366

Image not found
N-(4-Bromophenyl)urea
Measured: 260
Predicted: 256

Image not found
Benzoic acid, 2,4,5-trimethoxy-
Measured: 300
Predicted: 302